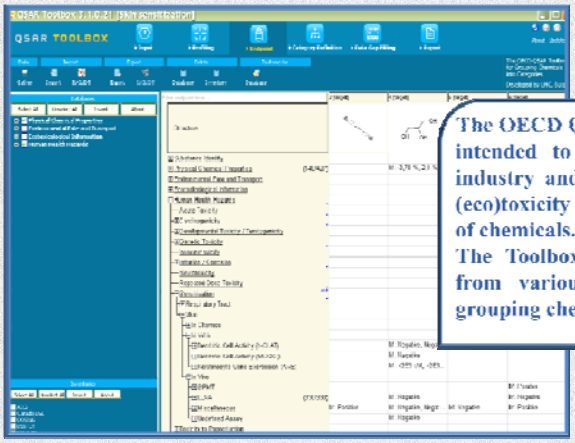
A Toxicological Ontology facilitates experimental databases mapping on the OECD Harmonised Templates' standard format

Olga Tcheremenskaia* (A), Romualdo Benigni (A), Monika Batke (B), George Fotakis (C) and Joop Deknecht (D)

(A) Istituto Superiore di Sanità (ISS), Environment and Health Department, Rome, Italy
(B) Fraunhofer Institute for Toxicology & Experimental Medicine (FITEM), Hannover, Germany
(C) European Chemicals Agency (ECHA), Assessment Unit, Helsinki, Finland
(D) Organization for Economic Co-operation and Development (OECD), Health and Safety Division, Paris, France



OECD QSAR Toolbox

The OECD QSAR Toolbox is a software application intended to be used by governments, chemical industry and other stakeholders in filling gaps in (eco)toxicity data needed for assessing the hazards of chemicals.
The Toolbox incorporates information and tools from various sources into a logical workflow, grouping chemicals into chemical categories

QSAR Toolbox 3.1 now available for free download
http://www.qsartoolbox.org/

Guidance documents, information and training materials, manuals
http://www.qsartoolbox.org/support.html

ECHA/OECD Ontology Program

The project started in 2012: ontologes for 6 toxicological endpoints will be release by the end of 2013.

Carcinogenicity Ontology - about 6000 terms (the Bio-Ontologies 2012 flash-update)

New Ontologies (July 2012-July 2013)

Repeated Dose Toxicity Ontology - about 20000 terms

Reproductive/Developmental Toxicity Ontology - about 34500 terms

Skin Irritation /Corrosion Ontology - about 1200 terms

Eye Irritation /Corrosion Ontology - about 1100 terms

Skin and Respiratory Sensitisation – work in progress, about 2000 terms will be collected

Sources for terms collection

-the OECD harmonised templates (standard data formats for reporting studies done on chemicals to determine their properties or effects on human health and the environment. http://www.oecd.org/ehs/templates/,
-OECD Test Guidelines,
-existing ontologies freely available at the Bioportal and OBO-Foundry ontology depositories:
(NCI Thesaurus, Clinical Terms Version 3 (CTV3), Mouse pathology, Mouse adult gross anatomy, Medical Dictionary for Regulatory Activities Terminology (MedDRA)),
-the toxicological ontology elaborated within the OpenTox project www.opentox.org
-experimental toxicological databases' terms

We use the DL species of the Web Ontology Language (OWL DL) supported by the Protégé OWL editor and the BioPortal import plug-in.

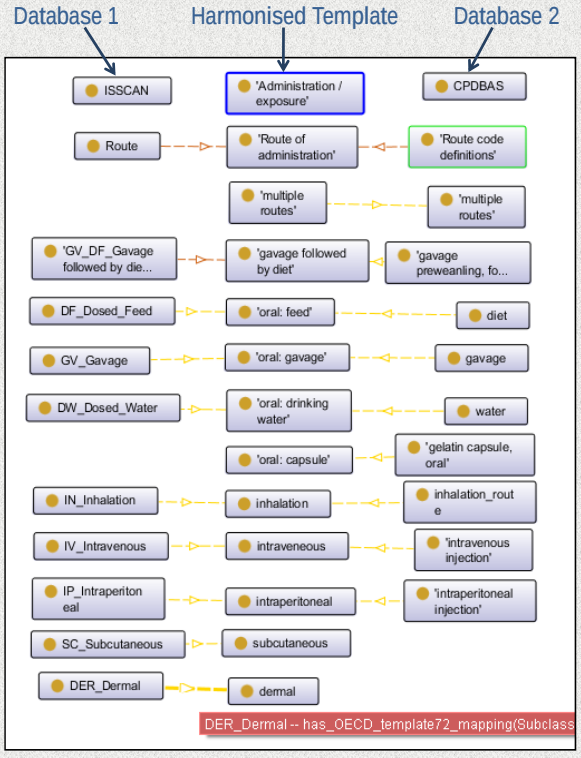
Why we need an ontology?

While the Toolbox is installed with a number of databases of experimental results.

The use of ontology will help to

-standardize the experimental terminology
-improve data integration
-remove uncertainties with synonyms,
-introduce the knowledge representation of toxicological data with
-possibility of automatic reasoning

Example of experimental data integration using ontology



OECD HT structure and ontology development principles?

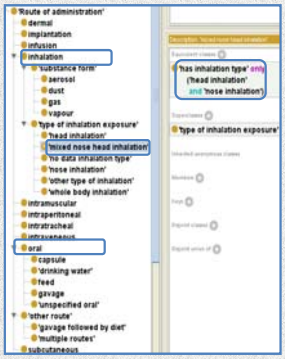
The regulatory toxicology terminology does not meet completely the principle of naming conventions.

We kept the original HT terminology and the structure of the HT's picklists (according to the contract).

Remodeling the hierarchy and names would destroy the harmonised templates structure.

Original structure

Possible changes



Acknowledgements

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